Linear, Multiple, and Logistic Regressions

CMPUT 328

Nilanjan Ray

Computing Science, University of Alberta, Canada

Linear regression with PyTorch

- We will start with a linear regression “model”
- Next, we need to understand “loss” function for regression task
- Next, we will estimate the model by minimizing the loss function
- We will use PyTorch

Supervised machine learning: the tabular view

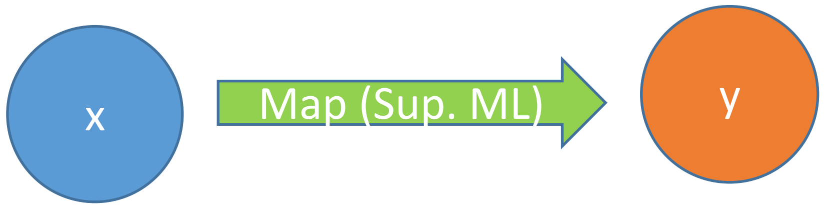
Independent variables (aka feature vector)

Prediction / dependent variable

x_1	x_2	x_3	x_4	y
1.2	-3.9	4.0	0	1.6
2.1	2.4	-0.7	-0.2	1.2
…	…	…	…	…
…	…	…	…	…
3.2	…	…	1.9	0.3
1.4	…	…	1.5	?
3.1	…	…	2.1	?

Training data: complete table

Test data: incomplete table



ML learns to map **x** to y

In other words, ML learns a function, *f* so that $y = f(\mathbf{x})$

The function *f* is called prediction function

Linear prediction: formal setup

Linear prediction function: $y^p = \mathbf{x}\boldsymbol{\theta} + b$ or, $y^p = \sum_{j=1}^{m} \theta_j x_j + b$

vector equation form

scalar equation form

A training set consists of ($\mathbf{x}$, y) pairs: $\{(\mathbf{x}_i, y_i)\}_{i=1}^{n}$

Linear prediction on the training data point *i*: $y_i^p = \mathbf{x}_i\boldsymbol{\theta} + b$ or, $y_i^p = \sum_{j=1}^{m} \theta_j x_{i,j} + b$

Loss or cost function (on training data): $L = \frac{1}{2}\sum_{i=1}^{n} (y_i^p - y_i)^2 = \frac{1}{2}\sum_{i=1}^{n} (\mathbf{x}_i\boldsymbol{\theta} + b - y_i)^2$

Learning the linear model: find out $\boldsymbol{\theta}$ and *b* to minimize loss function

Linear regression: A toy example

Let's take a toy example:

x_1	x_2	y
1	2	-1
3	-4	7
6	2	3
-3	5	-4
7	-3	5
4	3	?

This equation $y_i^p = \sum_{j=1}^{m} \theta_j x_{i,j} + b$

can be written for the toy training set as

$$
\begin{aligned}
y_1^p &= \theta_1(1) + \theta_2(2) + b \\
y_2^p &= \theta_1(3) + \theta_2(-4) + b \\
y_3^p &= \theta_1(6) + \theta_2(2) + b \\
y_4^p &= \theta_1(-3) + \theta_2(5) + b \\
y_5^p &= \theta_1(7) + \theta_2(-3) + b
\end{aligned}
$$

We also have ground truth responses:

$$y_1 = -1, y_2 = 7, y_3 = 3, y_4 = -4, y_5 = 5$$

So, the loss is $L = \frac{1}{2}\sum_{i=1}^{n} (y_i^p - y_i)^2 = \frac{1}{2}[(y_1^p + 1)^2 + (y_2^p - 7)^2 + (y_3^p - 3)^2 + (y_4^p + 4)^2 + (y_5^p - 5)^2]$

$$= \frac{1}{2}[(\theta_1 + 2\theta_2 + b + 1)^2 + (3\theta_1 - 4\theta_2 + b - 7)^2 + (6\theta_1 + 2\theta_2 + b - 3)^2 + (-3\theta_1 + 5\theta_2 + b + 4)^2 + (7\theta_1 - 3\theta_2 + b - 5)^2]$$

Learning a linear model

For the convenience of math, let us change our linear model a bit:

$$y_i^p = \sum_{j=1}^{m} \theta_j (x_{i,j} - \bar{x}_j) + b \quad \text{where} \quad \bar{x}_j = \frac{1}{n}\sum_{i=1}^{n} x_{i,j}$$

Subtracting independent variable mean is called “data centering”

Why? Because it simplifies the math later when solving for θ and b.

And a slightly modified loss function:

$$L = \underbrace{\frac{1}{2}\sum_{i=1}^{n} (y_i^p - y_i)^2}_{\text{Data fidelity}} + \underbrace{\frac{\gamma}{2}\sum_{j=1}^{m} \theta_j^2}_{\text{Regularization}}$$

γ is a hyper parameter

Why do we need regularization?

Minimization of linear regression loss function

Regularized loss function: $L = \frac{1}{2}\sum_{i=1}^{n}(y_i^p - y_i)^2 + \frac{\gamma}{2}\sum_{j=1}^{m}\theta_j^2$

Taking partial derivative using chain rule: $\frac{\partial L}{\partial b} = \sum_{i=1}^{n}(y_i^p - y_i)\frac{\partial y_i^p}{\partial b} = \sum_{i=1}^{n}(y_i^p - y_i)$ because, $\frac{\partial y_i^p}{\partial b} = 1$

Using $\bar{x}_j = \frac{1}{n}\sum_{i=1}^{n} x_{i,j}$ and $y_i^p = \sum_{j=1}^{m}\theta_j(x_{i,j} - \bar{x}_j) + b$ we get: $\frac{\partial L}{\partial b} = nb - \sum_{i=1}^{n} y_i$

At the minimum of *L*, $\frac{\partial L}{\partial b} = 0$ So, $b = \frac{1}{n}\sum_{i=1}^{n} y_i = \bar{y}$

Linear regression: A toy example...continued

Let's take a toy example:

x_1	x_2	y
1	2	-1
3	-4	7
6	2	3
-3	5	-4
7	-3	5
4	3	?

$$b = \frac{1}{n}\sum_{i=1}^{n} y_i = \bar{y} = \frac{1}{5}(-1+7+3-4+5) = 2$$

$$\bar{x}_1 = \frac{1}{n}\sum_{i=1}^{n} x_{i,1} = \frac{1}{5}(1+3+6-3+7) = 2.8$$

$$\bar{x}_2 = \frac{1}{n}\sum_{i=1}^{n} x_{i,2} = \frac{1}{5}(2-4+2+5-3) = 0.4$$

So, using centered data, the prediction equation becomes:

$$y_i^p = \sum_{j=1}^{m} \theta_j(x_{i,j} - \bar{x}_j) + b = \theta_1\left(x_{i,1} - 2.8\right) + \theta_2\left(x_{i,2} - 0.4\right) + 2$$

So, the loss is

$$L = \frac{1}{2}\sum_{i=1}^{n}(y_i^p - y_i)^2 = \frac{1}{2}\left[\left(y_1^p + 1\right)^2 + \left(y_2^p - 7\right)^2 + \left(y_3^p - 3\right)^2 + \left(y_4^p + 4\right)^2 + \left(y_5^p - 5\right)^2\right]$$

$$= \frac{1}{2}[(\theta_1(1-2.8) + \theta_2(2-0.4) + 2 + 1)^2 + (\theta_1(3-2.8) + \theta_2(-4-0.4) + 2 - 7)^2$$

$$+(\theta_1(6-2.8) + \theta_2(2-0.4) + 2 - 3)^2 + (\theta_1(-3-2.8) + \theta_2(5-0.4) + 2 + 4)^2 + (\theta_1(7-2.8) + \theta_2(-3-0.4) + 2 - 5)^2]$$

Minimization of linear regression loss function…

Regularized loss function:

$$L = \frac{1}{2}\sum_{i=1}^{n}(y_i^p - y_i)^2 + \frac{\gamma}{2}\sum_{j=1}^{m}\theta_j^2$$

Taking partial derivative of L using chain rule:

$$\frac{\partial L}{\partial \theta_j} = \sum_{i=1}^{n}(y_i^p - y_i)\frac{\partial y_i^p}{\partial \theta_j} + \gamma\theta_j$$

Using $\boxed{y_i^p = \sum_{k=1}^{m}\theta_k(x_{i,k} - \bar{x}_k) + b,}$ $\boxed{b = \bar{y}}$ and $\boxed{\frac{\partial y_i^p}{\partial \theta_j} = x_{i,j} - \bar{x}_j}$

We get: $$\frac{\partial L}{\partial \theta_j} = \sum_{i=1}^{n}\left(\sum_{k=1}^{m}\theta_k(x_{i,k} - \bar{x}_k) + \bar{y} - y_i\right)(x_{i,j} - \bar{x}_j) + \gamma\theta_j$$

Linear regression: A toy example…continued

Let's take a toy example:

x_1	x_2	y
1	2	-1
3	-4	7
6	2	3
-3	5	-4
7	-3	5
4	3	?

Note: For this toy problem, I assumed $\gamma = 0$ for convenience

$$\frac{\partial L}{\partial \theta_j} = \sum_{i=1}^{n} \left(\sum_{k=1}^{m} \theta_k (x_{i,k} - \bar{x}_k) + \bar{y} - y_i \right) (x_{i,j} - \bar{x}_j) + \gamma \theta_j$$

$$\begin{aligned}\frac{\partial L}{\partial \theta_1} &= (\theta_1(1-2.8) + \theta_2(2-0.4) + 2 + 1)(1-2.8) \\ &+ (\theta_1(3-2.8) + \theta_2(-4-0.4) + 2 - 7)(3-2.8) \\ &+ (\theta_1(6-2.8) + \theta_2(2-0.4) + 2 - 3)(6-2.8) \\ &+ (\theta_1(-3-2.8) + \theta_2(5-0.4) + 2 + 4)(-3-2.8) \\ &+ (\theta_1(7-2.8) + \theta_2(-3-0.4) + 2 - 5)(7-2.8) \\ &= (64.8)\theta_1 - (39.6)\theta_2 - 57\end{aligned}$$

$$\begin{aligned}\frac{\partial L}{\partial \theta_2} &= (\theta_1(1-2.8) + \theta_2(2-0.4) + 2 + 1)(2-0.4) \\ &+ (\theta_1(3-2.8) + \theta_2(-4-0.4) + 2 - 7)(-4-0.4) \\ &+ (\theta_1(6-2.8) + \theta_2(2-0.4) + 2 - 3)(2-0.4) \\ &+ (\theta_1(-3-2.8) + \theta_2(5-0.4) + 2 + 4)(5-0.4) \\ &+ (\theta_1(7-2.8) + \theta_2(-3-0.4) + 2 - 5)(-3-0.4) \\ &= (-39.6)\theta_1 + (57.2)\theta_2 + 63\end{aligned}$$

Minimization of linear regression loss function…

$$\frac{\partial L}{\partial \theta_j} = \sum_{i=1}^{n}\left(\sum_{k=1}^{m}\theta_k(x_{i,k}-\bar{x}_k)+\bar{y}-y_i\right)(x_{i,j}-\bar{x}_j)+\gamma\theta_j$$

$\Downarrow$ simplification

Gradient of *L* with resp. to $\boldsymbol{\theta}$:

$$\boxed{\nabla_{\boldsymbol{\theta}}L = \left[\sum_{i=1}^{n}(\mathbf{x}_i-\bar{\mathbf{x}})^T(\mathbf{x}_i-\bar{\mathbf{x}})\right]\boldsymbol{\theta}+\gamma\boldsymbol{\theta}-\sum_{\boldsymbol{i=1}}^{\boldsymbol{n}}(y_i-\bar{y})(\mathbf{x}_i-\bar{\mathbf{x}})^T}$$

where $\mathbf{x}_i = [x_{i,1} \quad \cdots \quad x_{i,m}]$, $\bar{\mathbf{x}} = [\bar{x}_1 \quad \cdots \quad \bar{x}_m]$ and $\boldsymbol{\theta} = [\theta_1 \quad \cdots \quad \theta_m]^T$

More simplified form: $\boxed{\nabla_{\boldsymbol{\theta}}L = (X^TX+\gamma I)\boldsymbol{\theta}-X^T\mathbf{y}}$

where matrix *X* is defined as: $X = \begin{bmatrix}\mathbf{x}_1-\bar{\mathbf{x}}\\ \vdots \\ \mathbf{x}_n-\bar{\mathbf{x}}\end{bmatrix}$ and vector $\mathbf{y}$ is defined as: $\mathbf{y} = \begin{bmatrix}y_1-\bar{y}\\ \vdots \\ y_n-\bar{y}\end{bmatrix}$

and *I* is an identity matrix of size *m*-by-*m*

Equating gradient of *L* to zero vector and solving for $\boldsymbol{\theta}$ gives us: $\boldsymbol{\theta} = (X^TX+\gamma I)^{-1}X^T\mathbf{y}$

Quick review: Gradient of a function

Consider a function of two variables as an example:

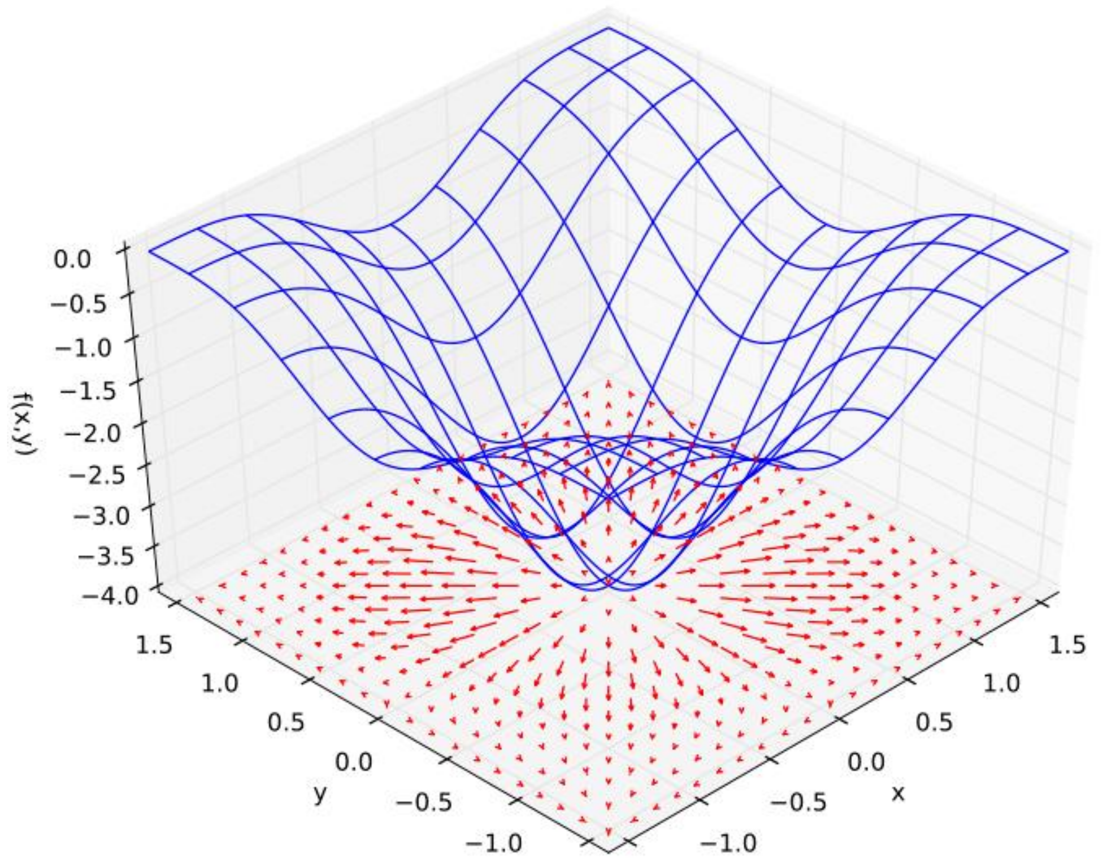
$$f(x,y) = -(cos^2 x + cos^2 y)^2$$

$$\nabla f(x,y) = \begin{bmatrix} \frac{\partial f}{\partial x} \\ \frac{\partial f}{\partial y} \end{bmatrix} = \begin{bmatrix} 4\left(cos^2(x) + cos^2(y)\right)\cos(x)\sin(x) \\ 4\left(cos^2(x) + cos^2(y)\right)\cos(y)\sin(y) \end{bmatrix}$$

Note 1: *f* is a function of two variables,
so gradient (partial derivatives collected as a vector)
of *f* is a two-dimensional vector

Note 2: Gradient (vector) of *f* points toward the
steepest ascent for *f*

Note 3: At a (local) minimum of *f* its gradient
becomes a zero vector



Example source: Wikipedia

Gradient in our toy example...

Toy example:

x_1	x_2	y
1	2	-1
3	-4	7
6	2	3
-3	5	-4
7	-3	5
4	3	?

$$\frac{\partial L}{\partial \theta_1} = (64.8)\theta_1 - (39.6)\theta_2 - 57$$

$$\frac{\partial L}{\partial \theta_2} = (-39.6)\theta_1 + (57.2)\theta_2 + 63$$

So, gradient is

$$\nabla L_{\boldsymbol{\theta}} = \begin{bmatrix} (64.8)\theta_1 - (39.6)\theta_2 - 57 \\ (-39.6)\theta_1 + (57.2)\theta_2 + 63 \end{bmatrix}$$

Equating gradient (vector) to 0 (vector) and solving, we get:

$$\boldsymbol{\theta} = \begin{bmatrix} \theta_1 \\ \theta_2 \end{bmatrix} = \begin{bmatrix} 0.3580 \\ -0.8535 \end{bmatrix}$$

Note: For this toy problem, I assumed $\gamma = 0$ for convenience

Equivalently, using direct formula…

Let's take a toy example:

x_1	x_2	y
1	2	-1
3	-4	7
6	2	3
-3	5	-4
7	-3	5
4	3	?

$$X = \begin{bmatrix} \mathbf{x}_1 - \bar{\mathbf{x}} \\ \vdots \\ \mathbf{x}_n - \bar{\mathbf{x}} \end{bmatrix} = \begin{bmatrix} 1-2.8 & 2-0.4 \\ 3-2.8 & -4-0.4 \\ 6-2.8 & 2-0.4 \\ -3-2.8 & 5-0.4 \\ 7-2.8 & -3-0.4 \end{bmatrix} \qquad \mathbf{y} = \begin{bmatrix} y_1 - \bar{y} \\ \vdots \\ y_n - \bar{y} \end{bmatrix} = \begin{bmatrix} -1-2 \\ 7-2 \\ 3-2 \\ -4-2 \\ 5-2 \end{bmatrix}$$

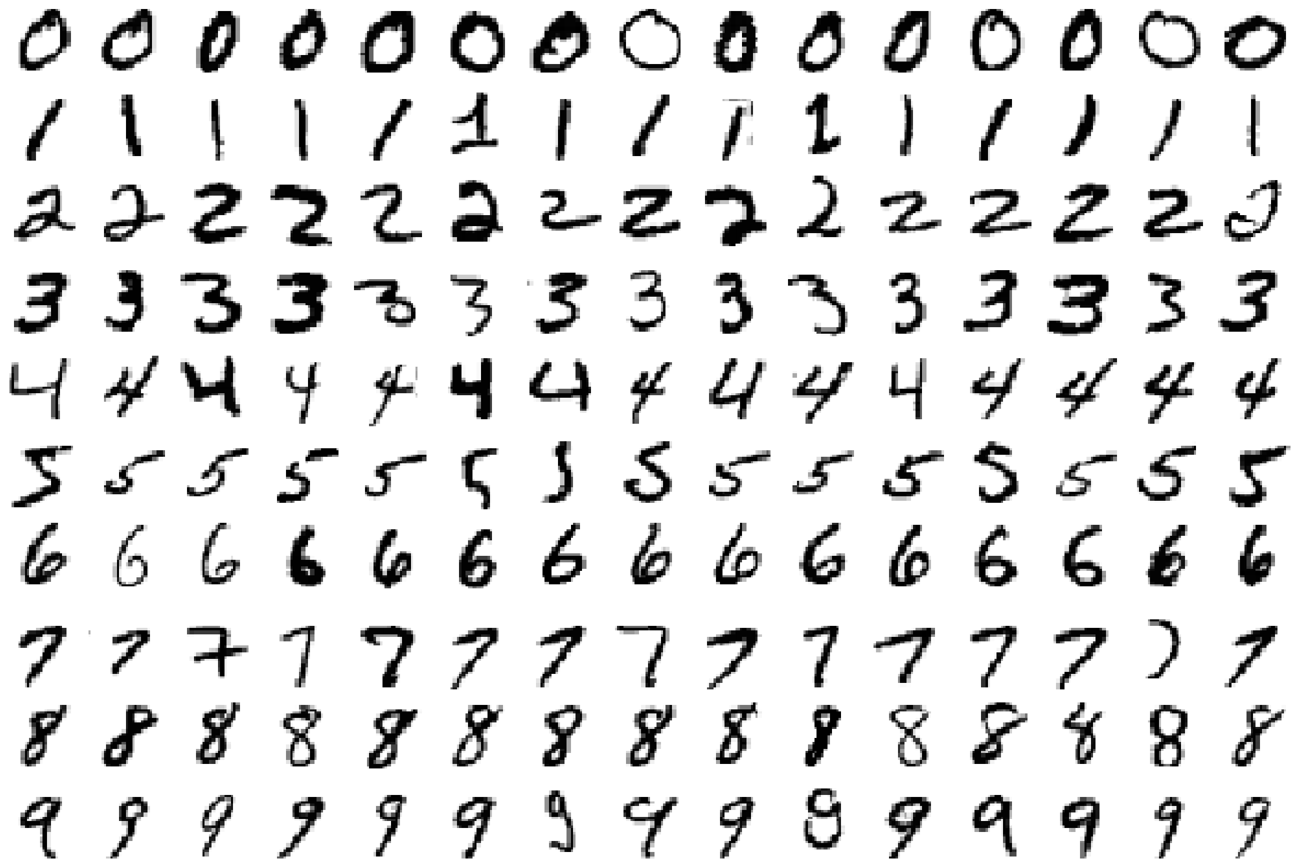
$$\boldsymbol{\theta} = (X^T X)^{-1} X^T \mathbf{y} = \begin{bmatrix} 0.3580 \\ -0.8535 \end{bmatrix}$$

So, finally the prediction for the test data point

$$? = \sum_{j=1}^{m} \theta_j (x_j - \bar{x}_j) + b = 0.3580(4-2.8) - 0.8535(3-0.4) + 2 = 0.2105$$

Note: For this problem I did not add any regularization, i.e., I assumed $\gamma = 0$

MNIST Dataset



Classify images into digits

Each image is **28x28**

10 labels

55,000 training images

5,000 validation images

10,000 test images.

Linear regression on MNIST dataset

Small 28 pixels-by-28 pixels images of hand written digits

The visual recognition problem definition:
to recognize the digit from an image

Our very first line of attack would be to use linear regression.

Feature dimension, m = 28 * 28 = 784

Let's look at our PyTorch implementations:
Called direct method because we will use math formula to find $\boldsymbol{\theta}$ and b.

Pixel values (feature)				Digit
x_1	x_2	…	x_{784}	y
0.1	0.3	…	0.0	0
0.2	0.1	…	0.5	1
…	…	…	…	…
…	…	…	…	…
0.0	0.98	…	0.8	9
0.5	0.25	…	0.36	?
0.1	0.95	…	0.1	?

Linear regression

So, far we have seen:

Image (1x784)

Parameters (784x1)

$$\mathbf{y}^p = (\mathbf{x} - \bar{\mathbf{x}})\,\theta + \bar{y} \longrightarrow$$

1 number, indicating digit

[28x28]
Array of real numbers
(784 numbers in total)

Mean vector of training images

Mean of training labels (digits)

Pixel values (feature) | Digit

x_1	x_2	...	x_{784}	y
0.1	0.3	...	0.0	0
0.2	0.1	...	0.5	1
...	...	...	...	...
...	...	...	...	...
0.0	0.98	...	0.8	9
0.5	0.25	...	0.36	?
0.1	0.95	...	0.1	?

See notebook: MNIST_Linear_Regression_Direct.ipynb

Multiple or Vector Linear Regression

[28x28]
Array of real numbers (784 numbers total)

Image (1x784)

Parameters (784x**10**)

$$\mathbf{y}^p = (\mathbf{x} - \bar{\mathbf{x}})\,W + \bar{\mathbf{y}}$$

Mean vector of training images

Mean of 1-hot training label vector

10 numbers, indicating class scores

Pixel values (feature)				Digit: 1-hot vector		
x_1	x_2	…	x_{784}	y_1	…	y_{10}
0.1	0.3	…	0.0	0	…	1
0.2	0.1	…	0.5	1		0
…	…	…	…	…	…	…
…	…	…	…	…	…	…
0.0	0.98	…	0.8	0	…	1
0.5	0.25	…	0.36	?	…	?
0.1	0.95	…	0.1	?	…	?

Multiple Linear Regression: PyTorch Implementation

See notebook: MNIST_Multiple_Linear_Regression_Direct.ipynb

Prediction model: $\mathbf{y}^p = (\mathbf{x} - \bar{\mathbf{x}})W + \bar{\mathbf{y}}$

https://en.wikipedia.org/wiki/Matrix_calculus

Regularized loss function: $L = \frac{1}{2}\sum_{i=1}^{n} \left\| \mathbf{y}_i^p - \mathbf{y}_i \right\|^2 + \frac{\gamma}{2}\|W\|^2$

This derivation requires matrix-vector differentiation

Gradient of loss function: $\boxed{\nabla_W L = (X^T X + \gamma I)W - X^T Y}$

where matrix *X* is defined as: $X = \begin{bmatrix} \mathbf{x}_1 - \bar{\mathbf{x}} \\ \vdots \\ \mathbf{x}_n - \bar{\mathbf{x}} \end{bmatrix}$

and matrix *Y* is defined as: $Y = \begin{bmatrix} \mathbf{y}_1 - \bar{\mathbf{y}} \\ \vdots \\ \mathbf{y}_n - \bar{\mathbf{y}} \end{bmatrix}$

and *I* is an identity matrix of size *784*-by-*784*

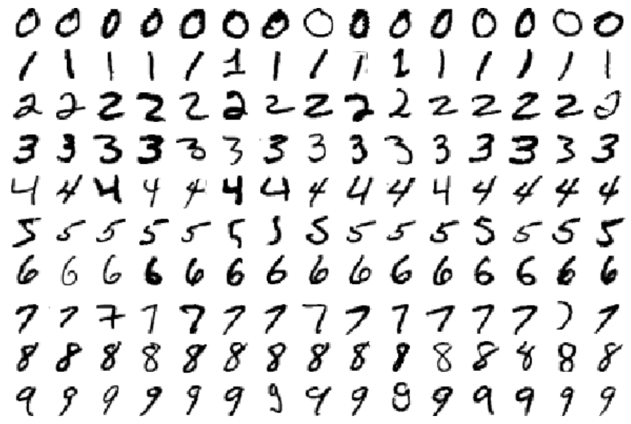
Equating gradient of *L* to zero matrix and solving for *W* gives us:

$$W = (X^T X + \gamma I)^{-1} X^T Y$$

We will “minimally” modify our linear regression scripts into multiple linear regression implementations!

What happened to our learning algorithm?

- Step 1: Create training image set (example set):



Repeat steps 2, 3 and 4

- Step 2: Show these examples to the machine learner
- Step 3: Measure mistakes made by the machine learner
- Step 4: Tune parameters of the machine learner to minimize its mistakes

Can we apply this learning algorithm to linear or multiple linear regression using PyTorch?

Iterate:

(Load Data): Get a training data batch (also called mini batch)

(Predict): Apply linear model to training feature vector and compute predictions

(Compute loss): Measure discrepancy between predictions and ground truths

(Optimize): Ask PyTorch to reduce loss value by tuning the parameters θ (or W), and b

(Diagnostics): Check if loss is decreasing

See notebook: MNIST_Linear_Regression.ipynb, MNIST_Multiple_Linear_Regression.ipynb

What are the pros and cons of this optimization-based method over the direct formula-based method?

Gradient descent optimization

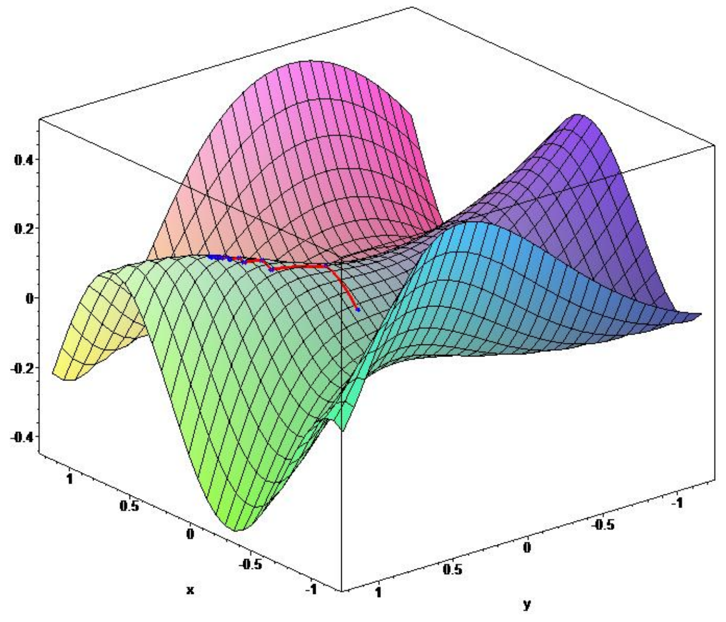
Start at an initial guess for the optimization variable: $\mathbf{x}_0$

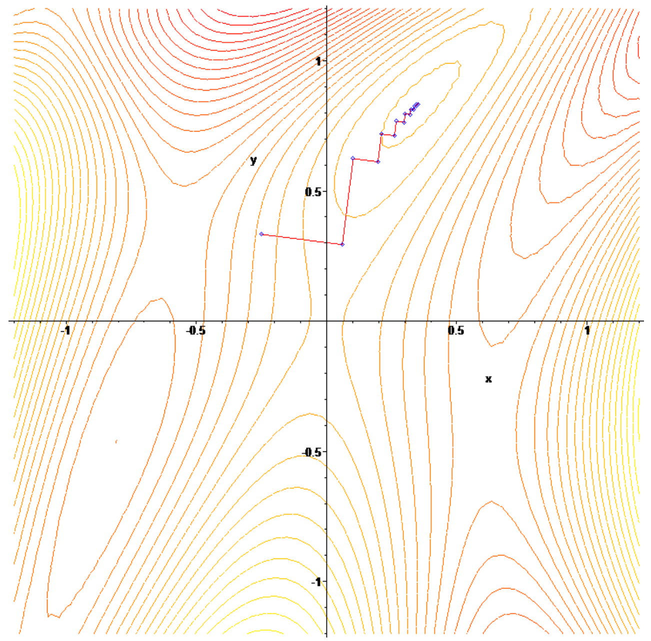
Iterate until gradient magnitude becomes too small: $\mathbf{x}^{t+1} = \mathbf{x}^t - \alpha \nabla f(\mathbf{x}^t)$

Gradient descent algorithm

α is called the step-length.

f(x, y)





Gradient descent creates a zig-zag path leading to a local minimum of f

Picture source: Wikipedia

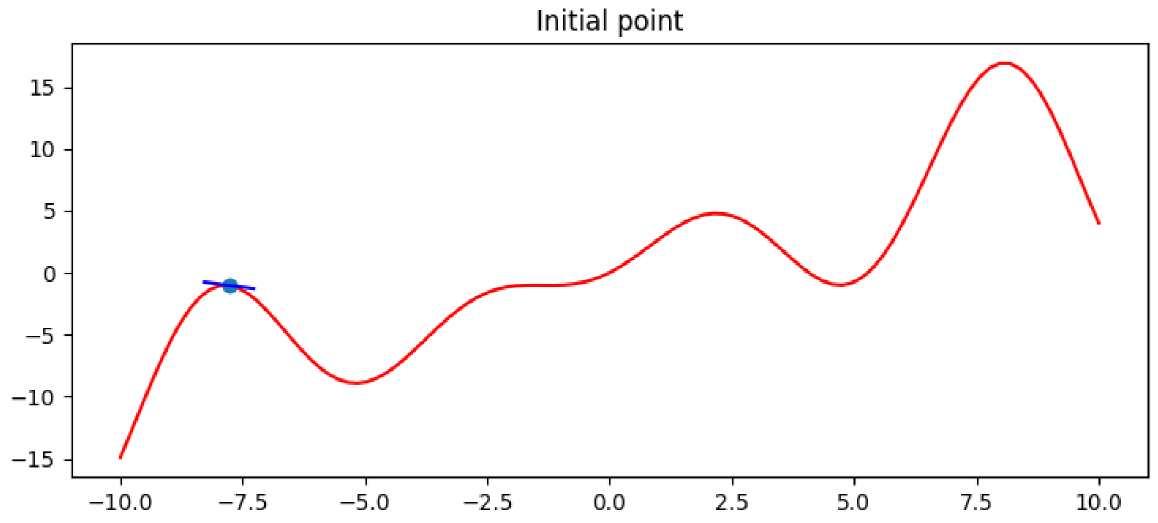
Gradient descent visualization

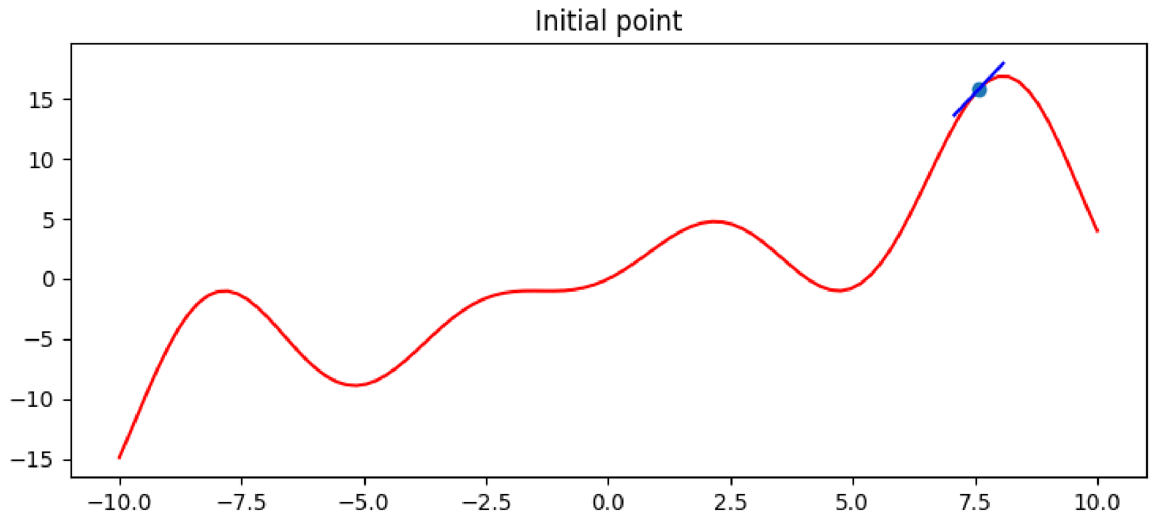
Find x such that f(x) is minimized: $f(x) = \sin(x) + x + x * \sin(x)$

$$\nabla f(x) = \cos(x) + 1 + \sin(x) + x * \cos(x)$$

$$\mathbf{x}_0 = ???$$

$$\mathbf{x}^{t+1} = \mathbf{x}^t - \alpha \nabla f(\mathbf{x}^t)$$





PyTorch optimizer uses GD

Let’s try our own gradient descent for multiple linear regression

Gradient of loss function for multiple linear regression: $\boxed{\nabla_W L = (X^T X + \gamma I)W - X^T Y}$

$$\boxed{\frac{\partial L}{\partial b} = \sum_{i=1}^{n} (y_i^p - y_i)}$$

Exercise: write GD for MNIST multiple linear regression

Look at MNIST_Multiple_Linear_Regression.ipynb

Logistic Regression

Can we modify scores from multiple regression function to output probabilities?

What is a suitable loss function for classification?

Logistic Regression

Would it not be nice if we can predict class probabilities instead of scores?

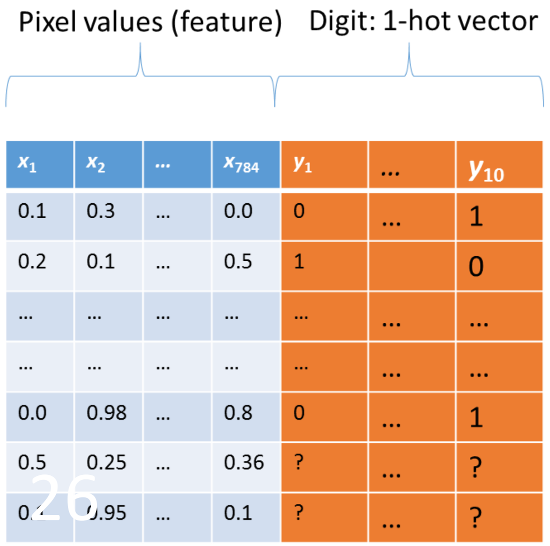
[28x28]
Array of real numbers
(784 numbers total)

image parameters

$$\mathbf{y}^p = f(\mathbf{x}, \mathbf{W}) \longrightarrow$$

prediction function
For logistic regression

10 numbers, indicating class probabilities



Pixel values (feature)				Digit: 1-hot vector		
x_1	x_2	…	x_{784}	y_1	…	y_{10}
0.1	0.3	…	0.0	0	…	1
0.2	0.1	…	0.5	1		0
…	…	…	…	…	…	…
…	…	…	…	…	…	…
0.0	0.98	…	0.8	0	…	1
0.5	0.25	…	0.36	?	…	?
[illegible]	0.95	…	0.1	?	…	?

Logistic regression: from multiple linear regression

Scores from multiple linear regression: $\mathbf{s}_i = (\mathbf{x}_i - \bar{\mathbf{x}})W + \bar{\mathbf{y}}$ or $\mathbf{s}_{i,k} = (\mathbf{x}_i - \bar{\mathbf{x}})W_{:,k} + \bar{\mathbf{y}}_k$

Score for *k*th class, *k* = 0,…,9

Predicted probability for *k*th class: $y_{i,k}^{p} = \frac{\exp(s_{i,k})}{\sum_{c=0}^{9}\exp(s_{i,c})}$

"Softmax" function

Logistic regression: loss function

Cross entropy loss: $loss(\mathbf{y}^p, \mathbf{y}) = -\sum_{k=0}^{9} \mathbf{y}_k \log(\boldsymbol{y}_k^p)$

Why this loss function? What does it mean? Why not use Euclidean loss as in MLR?

Do we have a direct formula to compute parameters like MLR?